Analysis of ^{238}Pu and ^{56}Fe Evaluated Data for Use in MYRRHA

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A sensitivity analysis on the multiplication factor, k_{eff}, to the cross section data has been carried out for the MYRRHA critical configuration in order to show the most relevant reactions. With these results, a further analysis on the ^{238}Pu and ^{56}Fe cross sections has been performed, comparing the evaluations provided in the JEFF-3.1.2 and ENDF/B-VII.1 libraries for these nuclides. Then, the effect in MYRRHA of the differences between evaluations are analysed, presenting the source of the differences. With these results, recommendations for the ^{56}Fe and ^{238}Pu evaluations are suggested. These calculations have been performed with SCALE6.1 and MCNPX-2.7e.

I. INTRODUCTION

The MYRRHA (Multi-purpose hYbrid Research Reactor for High-tech Applications) facility [1] is a flexible fast spectrum research reactor, conceived to work as an accelerator driven system (ADS) with a sub-critical configuration (at 70 MWth), or as a critical reactor (100 MWth). It is cooled with Lead-Bismuth Eutectic (LBE), which also is used as the spallation target for the sub-critical configuration. The MYRRHA driver fuel is MOX containing 30 % of plutonium.

The verification and validation of a neutronics analysis code and set of nuclear data is an important part of the licensing process. Once a code and set of data are selected, they will be used in all neutronics calculations related to safety for a very long period of time. Therefore, a comparison of codes and nuclear data libraries should be performed. In this case, an sensitivity and uncertainty (S/U) analysis can help us to focus on the most relevant reactions for e.g. criticality calculations in order to compare nuclear data libraries and neutronic codes.

An S/U analysis for criticality calculations of the previous MYRRHA design, XT-ADS, was reported recently [2] where the effect between using different libraries is also studied. This study has recently been updated for the new MYRRHA core layout in [3]. However, the origin of the differences between using one library or the other was not studied in either of the previous works.

Therefore, this paper is aimed first to perform a new sensitivity analysis of the neutron multiplication factor, k_{eff}, to the cross section data for the current MYRRHA design, using SCALE6.1 [4]. Once the importance of the reactions are ranked, the cross section data from the ENDF/B-VII.1 [5] and JEFF-3.1.2 [6] libraries are compared for the most relevant reactions for MYRRHA of ^{56}Fe and ^{238}Pu . Finally, the impact on the criticality calculations of the differences between cross sections is assessed using the MCNPX-2.7e [7] code.

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II. SENSITIVITY ANALYSIS OF MYRRHA TO CROSS SECTION DATA

The SCALE6.1 suite [4] is chosen for performing the sensitivity analysis of k_{eff} to the cross section data for the critical configuration of the MYRRHA design, as done before for XT-ADS [2]. The SCALE modules used are: KENO-VI, which performs the forward and adjoint transport calculations; and SAMS, which calculates the sensitivity coefficients applying linear perturbation theory.

The MYRRHA critical core studied and implemented in SCALE consists of 57 Fuel Assemblies (FAs), 6 Control Rod assemblies (CR), 3 Scram Rod assemblies (SR), 7 In-Pile Sections (IPSs), surrounded first by LBE dummy assemblies, and then by reflector assemblies (YZrO). The geometrical model is presented in Fig. 1. The FAs are modelled in detail, while the rest of the elements are represented by homogenized hexagonal cells of the materials within the cell.

The sensitivity analysis provides two different values to assess the importance of the cross sections: *Sensitivity coefficients*, $\frac{\partial k_{eff}}{k_{eff}} / \frac{\partial \sigma_i}{\sigma_i}$, which measure how the k_{eff} value will change if the energy-group cross section is modified; *Integrated Sensitivity Coefficients* (ISC), which are the sums over the whole energy range of the sensitivity coefficients of one cross section. The former is used to analyse

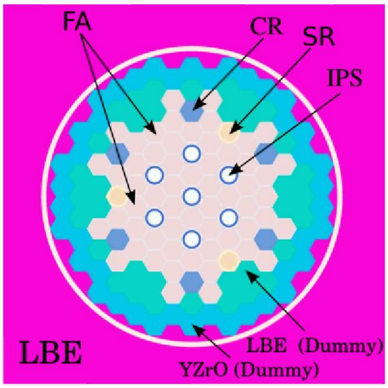

FIG. 1. MYRRHA model for the critical configuration, implemented in KENO-VI (SCALE6.1).

in which energy range the cross sections are of importance, while the latter represents within a single value the absolute relevance of the reaction.

Table I ranks the importance of each reaction involved in the MYRRHA neutronic model by their ISC values. These values are compared with the ones obtained in XT-ADS [2]. Very similar results are observed between both designs, because the neutron spectrum is almost the same. The elastic reactions, however, are in disagreement. Fission, capture and average prompt fission neutron multiplicity ($\bar{\nu}$) reactions of ^{238}U and ^{239,240,241}Pu are the most important. However, the reaction of a non-actinide isotope is also of relevance: ^{209}Bi(n,n). The three most important reactions for ^{56}Fe and ^{238}Pu are presented at the bottom of the table. Again, for the ^{56}Fe(n,n) reaction, a large difference (note the different signs of the effect) is observed between MYRRHA and XT-ADS. All these results confirm the findings drawn from Ref. [3].

For the ^{56}Fe and ^{238}Pu reactions shown in Table I, their sensitivity profiles are presented in Fig. 2. ^{56}Fe(n,n) and (n,γ) reactions are relevant from low to high energies, specially due to the resonance at 1.151 keV [6] / 1.1497 [5]. Meanwhile, ^{238}Pu reactions are of importance at high energies, above 0.5 keV.

III. IMPACT OF DIFFERENT NUCLEAR DATA LIBRARIES ON MYRRHA CRITICALITY CALCULATIONS

The evaluations in ENDF/B-VII.1 [5] and JEFF-3.1.2 [6] are compared for ^{56}Fe and ^{238}Pu . The impact of these evaluations in MYRRHA criticality calculations is assessed by substituting the whole or parts of JEFF-3.1.2, with the ones in ENDF/B-VII.1 for ^{56}Fe first, and then for ^{238}Pu . Meanwhile, for the rest of isotopes the JEFF-3.1.2 library is used. The effect of using one library or the other has been analysed previously in Ref. [3], however, the analysis of the impact of the different reactions of these two isotopes is performed here.

TABLE I. The first 12 cross section Integrated Sensitivity Coefficients (ISC) for MYRRHA sorted in decreasing order of its absolute value, and compared with XT-ADS results [2]. The three largest ISC of ^{56}Fe and ^{238}Pu are presented.

		MYRRHA		XT-ADS
Isotope	Reaction	ISC	Std.Dev. [a]	ISC
^{239}Pu	$\bar{\nu}$	6.97×10^{-1}	0.01%	7.06×10^{-1}
^{239}Pu	(n,f)	4.78×10^{-1}	0.01%	4.71×10^{-1}
^{241}Pu	$\bar{\nu}$	1.04×10^{-1}	0.01%	1.04×10^{-1}
^{238}U	(n,γ)	-1.02×10^{-1}	0.02%	-1.02×10^{-1}
^{240}Pu	$\bar{\nu}$	8.26×10^{-2}	0.01%	8.38×10^{-2}
^{241}Pu	(n,f)	7.12×10^{-2}	0.01%	6.89×10^{-2}
^{238}U	$\bar{\nu}$	6.13×10^{-2}	0.02%	5.53×10^{-2}
^{239}Pu	(n,γ)	-5.76×10^{-2}	0.03%	-5.98×10^{-2}
^{240}Pu	(n,f)	5.58×10^{-2}	0.02%	5.68×10^{-2}
^{209}Bi	(n,n)	5.04×10^{-2}	0.30%	1.50×10^{-2}
^{238}U	(n,f)	3.77×10^{-2}	0.04%	3.46×10^{-2}
^{240}Pu	(n,γ)	-2.56×10^{-2}	0.03%	-2.71×10^{-2}
^{56}Fe	(n,n)	2.21×10^{-2}	1.28%	-6.71×10^{-3}
	(n,γ)	-1.41×10^{-2}	0.02%	-1.97×10^{-2}
	(n,n')	-7.33×10^{-3}	0.96%	-4.92×10^{-3}
^{238}Pu	$\bar{\nu}$	1.96×10^{-2}	0.01%	1.99×10^{-2}
	(n,f)	1.35×10^{-2}	0.01%	1.35×10^{-2}
	(n,γ)	-3.51×10^{-3}	0.04%	-3.70×10^{-3}

[a] Std.Dev.= Standard deviation of the statistical uncertainty.

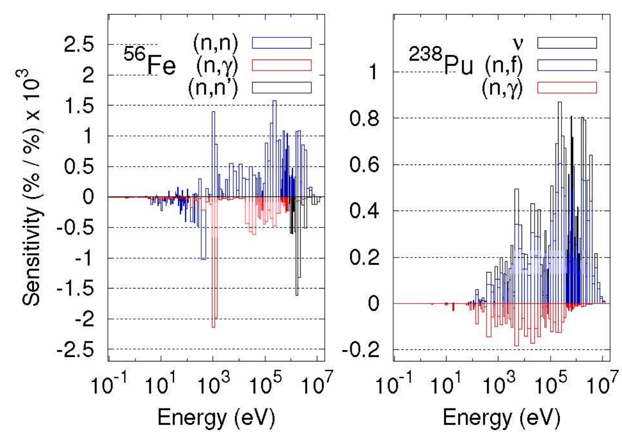

FIG. 2. Sensitivity profiles of the three most important reactions of ^{56}Fe and ^{238}Pu .

A. ^{56}Fe

The ENDF/B-VII.1 evaluation for ^{56}Fe is based on the one performed for ENDF/B-VI.1 [8], while JEFF-3.1.2 takes the ^{56}Fe evaluation from EFF-3.1 (European Fusion File 3.1 - Jan 2001). The relevant differences between these two evaluations for (n,γ) and (n,n) reactions lie below 850 keV, where cross sections are defined mainly by resonance parameters. There, ENDF/B-VI.1 provides a background cross section for (n,γ), which is added to the

TABLE II. Summary of MCNPX criticality calculations for the critical configuration of MYRRHA at BOL, where the ^{56}Fe and ^{238}Pu cross section files are changed or modified.

^{56}Fe base file	Modified part [a]	k_{eff}	Δk_{eff} (pcm)
JEFF-3.1.2	-	1.05374±0.00008	-
ENDF/B-VII.1	-	1.05224±0.00008	-142.35
JEFF-3.1.2	(n,n)	1.05343±0.00007	-29.42
JEFF-3.1.2	(n,γ)	1.05275±0.00008	-93.95

^{238}Pu base file	Modified part [a]	k_{eff}	Δk_{eff} (pcm)
JEFF-3.1.2	-	1.05363±0.00008	-
ENDF/B-VII.1	-	1.05178±0.00008	-175.58
JEFF-3.1.2	$\overline{\nu}$	1.05378±0.00008	14.24
JEFF-3.1.2	(n,f)	1.05201±0.00008	-153.75
JEFF-3.1.2	(n,γ)	1.05319±0.00008	-41.760

[a] Modified parts are substituted with the ones in ENDF/B-VII.1

cross section calculated with the resonance parameters. On the other hand, EFF-3.1 provides more resonances for which at least two, at 423.1 keV and 446.0 keV, are not found in the literature. The ENDF/B-VI.1 evaluation provides higher cross section values than EFF-3.1 because of the background cross section. Based on the sensitivity profile given in Fig. 2, one can expect the effect of these differences to be of relevance. This is indeed shown in Table II in the line where only the (n,γ) cross section in JEFF-3.1.2 is substituted with the ENDF/B-VII.1 one. As can also been seen from this table, the differences in the (n,γ) cross section are more relevant that the differences for (n,n).

B. ^{238}Pu

For ENDF/B-VII.1, a new evaluation was made in September 2010, which takes the resonance parameters from JENDL-4.0 [9]. JEFF-3.1.2 takes the evaluation made in JENDL-3.2 [10], but for the Unresolved Resonance Region (URR) the cross sections from the BROND-2.2 evaluation are taken. Both libraries, ENDF/B-VII.1 and JEFF-3.1.2, take parts of their evaluations of ^{238}Pu from JENDL, so small differences are expected to be found. However, the usage of part of the BROND-2.2 evaluation for ^{238}Pu by JEFF-3.1.2 in URR is responsible for the most relevant differences. For (n,γ), BROND-2.2 makes JEFF-3.1.2 to provide smaller values than ENDF/B-VII.1 between 3 keV and 150 keV while for (n,f) the trend is inverted. Again, these differences lie in the region where the sensitivity coefficients to these two cross sections (Fig. 2) are high. As such the effect of substituting (n,f) and (n,γ) cross sections of JEFF-3.1.2 with the ENDF/B-VII.1 counterparts is expected to be important. This confirms the values reported in Table II. The major effect is caused by the (n,f) reaction, which almost covers all the difference that comes from changing the whole library.

IV. CONCLUSIONS

A sensitivity analysis has been done for the critical configuration of MYRRHA with SCALE6.1 suite. The most relevant reactions have been highlighted, confirming the main results drawn in Ref. [3]. Special attention has been paid to ^{56}Fe and ^{238}Pu cross sections, remarking the most important reactions. The differences between the evaluations of ^{56}Fe and ^{238}Pu used in ENDF/B-VII.1 and JEFF-3.1.2 are analysed. They help to clarify where the differences obtained between using one evaluation instead of the other in the criticality calculations for MYRRHA come from.

Therefore, under the MYRRHA framework, a review on the usage of background cross sections or unreal resonance parameters for ^{56}Fe is suggested. Because of the age (more than 20 years) of the ^{56}Fe evaluation used in ENDF/B-VII.1, maybe a new evaluation could be performed. Regarding ^{238}Pu , ENDF/B-VII.1 seems to be more reliable than JEFF-3.1.2, because a new evaluation for ^{238}Pu is used. JEFF-3.1.2 should question the usage of the BROND-2.2 evaluation throughout the Unresolved Resonance Region (URR), which makes (n,γ) reaction being underestimated, and (n,f) overestimated.

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